

# Symmetry breaking by the sea of Dirac-Landau levels in graphene

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(Dated: February 1, 2008)

The quantum Hall states of graphene have a filled sea of lower Dirac-Landau levels. The short ranged  $SU(4)$  symmetry breaking interactions can induce a staggered polarization of the sea of Dirac-Landau levels. We study this effect in the extended Hubbard model on a honeycomb lattice using mean field variational wavefunctions. We find a valley symmetry broken, anti-ferromagnetic spin ordered phase at  $\nu = \pm 1$  when the on-site interaction is dominant. Our mean field solution is consistent with the recently reported experimental results of Z. Jiang et. al.[1]

The low energy physics of graphene is described by quasiparticles satisfying the massless Dirac equation [2] [3]. There are two species of Dirac fermions per spin making a total of four species of quasiparticles. In the non-interacting limit, these four species are degenerate resulting in an  $SU(4)$  symmetry of the non-interacting theory. The dominant interaction is the long-range part of the Coulomb interaction which is also  $SU(4)$  symmetric.

The quantum Hall effect has been observed in graphene [1] [2] [3] [4] [5]. At low magnetic fields ( $\sim 1-10$  T), plateaus are observed at  $(h/e^2)\sigma_H = 4(n + 1/2)$  consistent with there being four degenerate Dirac-Landau levels. At higher fields ( $\sim 20-45$  T), this degeneracy is lifted [5]. It is completely lifted in the  $n = 0$  level resulting in extra plateaus at  $(h/e^2)\sigma_H = -1, 0, 1$  and partially lifted for  $n = \pm 1$  yielding extra plateaus at  $(h/e^2)\sigma_H = \pm 4$ . Tilted field experiments [5] indicate that the plateau at  $(h/e^2)\sigma_H = \pm 4$  is due to the Zeeman splitting of the Landau levels. Recent experiments by Z. Jiang et. al. [1] show that the transport gap at the  $(h/e^2)\sigma_H = \pm 1$  ( $\nu = \pm 1$ ) plateau does not depend on the parallel component of the magnetic field and is proportional to  $\sqrt{B_\perp}$ . These experiments hence indicate that the  $\nu = \pm 1$  plateau corresponds to a state with zero net spin polarisation. These plateaus are attributed to the lifting of the sub-lattice degeneracy of the  $n = 0$  Landau level.

It has been shown that the long range part of the Coulomb interaction causes the  $SU(4)$  symmetry to be broken spontaneously [6] [7] [8] [9]. The resulting gap is proportional to  $\sqrt{B_\perp}$ . The exact pattern of the symmetry breaking is not determined by the  $SU(4)$  symmetric long range part of Coulomb interaction but by other symmetry breaking interactions [10]. These could be the

Zeeman term, short range lattice scale interactions [11] [8] [12] and disorder [13]. The effects of the short range lattice scale interactions can be studied in the extended Hubbard model on the honeycomb lattice in the presence of a magnetic field. The previous studies of this model [8][11] find a spin polarised state at  $\nu = \pm 1$ . However, this is not consistent with the experiments discussed above [1].

In this work, we are mainly concerned with the physics of  $\nu = \pm 1$  states and we show that the sea of Dirac-Landau levels plays a significant role. We write down mean field trial wavefunctions that incorporate a staggered  $SU(4)$  polarization of the  $n \neq 0$  Landau levels and compute their energies analytically in a systematic  $a/l_c$  expansion [9], where  $a$  ( $= 2.45$  Å) is the lattice spacing and  $l_c$  ( $\approx 40$  Å at 45 T) is the magnetic length. We then find that when the on-site repulsion is dominant, the ground state has anti-ferromagnetic ordering with broken valley symmetry. It has zero net spin polarisation and hence is a strong candidate for the state found in the experiments [1].

The hamiltonian we consider is,

$$\mathcal{H} = -t \sum_{\langle ij \rangle, \sigma} \left( e^{i\phi_{ij}} c_{i\sigma}^\dagger c_{j\sigma} + h.c \right) + \frac{U}{2} \sum_i (\hat{n}_i - 1)^2 + V \sum_{\langle ij \rangle} (\hat{n}_i - 1)(\hat{n}_j - 1) \quad (1)$$

$\hat{n}_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$  is the number operator and  $\phi_{ij}$  is the phase due to presence of the magnetic field. The continuum model describing the low energy physics can be derived in the standard way. The continuum effective hamiltonian is,

$$\mathcal{H} = \int d^2x \Psi^\dagger (v_F \boldsymbol{\alpha} \cdot \boldsymbol{\Pi}) \Psi - \frac{Ua^2}{12} \left( (\Psi^\dagger \sigma^a \Psi)^2 + (\bar{\Psi} \tau^z \sigma^a \Psi)^2 + \frac{1}{2} (\Psi^\dagger \alpha^i \tau^j \sigma^a \Psi)^2 \right) + \frac{3Va^2}{4} \left( (\Psi^\dagger \Psi)^2 - (\bar{\Psi} \tau^z \Psi)^2 \right) \quad (2)$$

Where  $\boldsymbol{\Pi}$  is the covariant derivative. The kinetic en-

ergy term has an  $SU(4)$  internal symmetry whereas the

interaction terms break it down to  $(Z_2 \rtimes U(1))_{valley} \otimes SU(2)_{spin}$ . The remanent of the  $SU(2)$  valley symmetry of the non-interacting theory corresponds to

$$\Psi_{r\eta\sigma}(\mathbf{x}) \rightarrow \tau_{\eta\bar{\eta}}^x \Psi_{r\bar{\eta}\sigma}(\mathbf{x}) \quad (3)$$

$$\Psi_{r\eta\sigma}(\mathbf{x}) \rightarrow \left( e^{i\theta\tau^z} \right)_{\eta\bar{\eta}} \Psi_{r\bar{\eta}\sigma}(\mathbf{x}) \quad (4)$$

where,  $r$  is the Dirac (sub-lattice) index,  $\eta$  the valley index and  $\sigma$  the spin index. Note that the  $Z_2$  does not commute with the  $U(1)$ . The  $Z_2$  part of the valley symmetry corresponds to the interchanging of the valley indices. The  $U(1)$  part corresponds to the conservation of the number of quasiparticles belonging to the two valleys separately. This is a symmetry only of the low energy sector as scattering from one valley to the other is a high momentum transfer process. There are also no Umklapp processes which contribute to this process.

Our variational wavefunctions generalise those written down by Yang et. al. [7] to include the polarisation of the Dirac sea. They are constructed from the eigenfunctions of the following massive single particle Dirac equation,

$$h = v_F \boldsymbol{\alpha} \cdot \boldsymbol{\Pi} + \beta m Q \quad (5)$$

where  $m$  is a real number and  $Q$  a matrix constructed from a basis of four orthonormal  $SU(4)$  spinors,

$$Q = \sum_{p=1}^k \chi^p (\chi^p)^\dagger - \sum_{p=k+1}^4 \chi^p (\chi^p)^\dagger \quad (6)$$

for the case where  $k$  of the four  $n = 0$  levels are occupied.

The variational states are,

$$|k\rangle = \left( \prod_{p=1}^k \prod_l \psi_{0lp}^\dagger \right) \left( \prod_{n=-N_c}^{-1} \prod_{lp} \psi_{nlp}^\dagger \right) |0\rangle \quad (7)$$

where,

$$\Psi(\mathbf{x}) = \sum_{nlp} \Phi^{nl}(\mathbf{x}) \chi^p \psi_{nlp} \quad (8)$$

$\Phi^{nl}(\mathbf{x}) \chi^p$  being the eight component spinor eigenfunctions of the hamiltonian in Eq.(5). The cutoff on the number of Landau levels,  $N_c$ , is obtained by matching the total number of states with that of the lattice. We have,  $N_c = (2\pi/\sqrt{3})(l_c^2/a^2)$ . Note that in the limit  $m \rightarrow 0$ , our variational states reduce to those of Yang et. al. [7]. The ground state manifold is  $U(4)/(U(k) \times U(4-k))$  for all  $m$ . The single particle energy levels are shifted by the presence of the mass term as shown in Fig.(1).

For the computation of the expectation value of the hamiltonian, we need to compute the coincident two point correlation function

$$\Gamma = \sum_{nlp \in occ} \langle (\Phi^{nlp}(\mathbf{x}))^\dagger \Phi^{nlp}(\mathbf{x}) \rangle \equiv \sum_{n=-N_c}^0 \Gamma^n$$



FIG. 1: (a) shows the energy levels for non-interacting Dirac particles in magnetic field for graphene.(b) shows the shift in one particle levels due to mass and the filling of one particle states for  $\nu = -1$ .

Assuming that  $m \sim (a/l_c)^2$  we put  $m = \tilde{m}(a^2/(2\pi l_c^2))$ . This assumption will be justified later when we solve for  $m$ .  $\Gamma^n$  can be computed to leading order in  $a/l_c$  to be,

$$\Gamma^0 = \frac{1}{2\pi l_c^2} \frac{1-\beta}{2} \frac{1+Q}{2} \quad (9)$$

$$\Gamma^n = \frac{1}{2\pi l_c^2} \left( \frac{1}{2} + \frac{\beta}{2} \frac{a}{2\pi l_c} \text{sgn}(n) \frac{\tilde{m} Q}{\sqrt{3t} \sqrt{2|n|}} \right), n \neq 0 \quad (10)$$

Equation (10) shows that the mass term induces a staggered  $SU(4)$  polarization of the  $n \neq 0$  Landau levels. Since the Dirac index is the same as the sub-lattice index, the order parameters for staggered  $SU(4)$  order are  $\langle \bar{\Psi} \lambda^a \Psi \rangle = \text{Tr } \beta \lambda^a \Gamma$ , where  $\lambda^a$  are the  $SU(4)$  generators.

Using the two point coincident correlation function we can compute the expectation values of hamiltonian in terms of  $Q$  the matrix. The kinetic energy density,  $E_t$ , interaction energy densities  $E_V$  and  $E_U$  are computed to be, (here we have retained the terms upto leading order in  $a/l_c$  and dropped the terms that are independent of  $m$  and  $Q$ )

$$E_t = \frac{1}{2\pi l_c^2} \frac{a^2}{2\pi l_c^2} \frac{2\tilde{m}^2}{t} \quad (11)$$

$$E_V = \frac{1}{2\pi l_c^2} \frac{a^2}{2\pi l_c^2} \frac{3V}{4} \left( -\frac{\mu^2}{2} - \frac{\mu^2}{4} (\text{Tr}(\tau^z Q))^2 + \frac{\mu^2 + 1}{8} \text{Tr}(\tau^z Q \tau^z Q) \right) \quad (12)$$

$$E_U = \frac{1}{2\pi l_c^2} \frac{a^2}{2\pi l_c^2} \frac{U}{12} \left( \frac{1}{4} (\text{Tr}(\sigma^a Q))^2 - \frac{\mu^2 + 1}{8} \text{Tr}(\sigma^a Q \sigma^a Q) + \frac{\mu^2}{4} (\text{Tr}(\tau^z \sigma^a Q))^2 - \frac{\mu^2 + 1}{8} \text{Tr}(\tau^z \sigma^a Q \tau^z \sigma^a Q) + \frac{\mu^2 - 1}{8} \text{Tr}(\tau^j \sigma^a Q \tau^j \sigma^a Q) \right) \quad (13)$$

where,  $\mu \equiv 1 + (2\tilde{m}/\tilde{t})$  and  $\tilde{t} \equiv (t/2)(3\sqrt{3}\pi)^{1/2}$ . Note that the  $m \rightarrow 0$  limit is obtained by putting  $\mu = 1$  i.e. the contribution of filled sea of Dirac-Landau levels is neglected to the mean field energy.

We now specialise to the case when  $\nu = -1$  ( $k = 1$ ) where a single  $n = 0$  Dirac-Landau level is filled. The ground state manifold is parametrised by a single  $SU(4)$  spinor which specifies the  $SU(4)$  polarization. The  $\nu = 1$  ( $k = 3$ ) case is related to the former by a particle-hole transformation. We use an explicit parameterisation,

$$|\chi\rangle = \cos \frac{\gamma}{2} |+\rangle |\hat{n}_1\rangle + e^{i\Omega} \sin \frac{\gamma}{2} |-\rangle |-\hat{n}_2\rangle \quad (14)$$

This corresponds to a linear superposition of an electron with valley index  $+$ , spin polarization  $\hat{n}_1$  and valley index  $-$ , spin polarization  $-\hat{n}_2$ .  $\gamma$  and  $\Omega$  specify the relative amplitude and phase of the superposition.

When the  $\gamma$  is either 0 or  $\pi$  the many body state has a definite number of electrons in each valley. The  $n = 0$  level electrons are localised in one sub-lattice with arbitrary spin, corresponding to charge and spin ordering. These are the states discussed in previous work [8][11]. They have the  $U(1)$  part of the valley symmetry unbroken and the  $Z_2$  part broken.

When  $0 < \gamma < \pi$ , the many body state does not have a definite number of electrons in each valley. The total number however, remains a good quantum number. Further, if  $\gamma \neq \pm\pi/2$ , then the average number of electrons in each valley is not the same and there is charge ordering. In this case the full valley symmetry,  $Z_2 \rtimes U(1)$ , is broken. When  $\gamma = \pm\pi/2$ , the average number of electrons in the two valleys are equal, the  $Z_2$  symmetry is unbroken and the  $U(1)$  is broken.

In general the state will have a non-zero total spin polarization except when  $\gamma = \pm\pi/2$  and  $\hat{n}_1 = \hat{n}_2$ . In this case there is anti-ferromagnetic spin order and no charge order.

We now evaluate the energy density in terms of our parameters by substituting Eq.(14) in equations (6,12 and 13). The total mean field energy density ( $E$ ) is the sum of kinetic ( $E_t$ ), nearest neighbour interaction ( $E_V$ ), Hubbard interaction ( $E_U$ ) and Zeeman term ( $E_Z$ ).

$$E = \frac{1}{2\pi l_c^2} \frac{a^2}{2\pi l_c^2} \left( \frac{2\tilde{m}^2}{\tilde{t}} - \frac{3}{4}V \left( \frac{1}{2} + \frac{\mu^2 - 1}{2}(1 + \cos^2 \gamma) \right) - \frac{1}{16}U((\mu^2 - 1)(1 + \cos \theta) \sin^2 \gamma) - \tilde{g} \frac{2\pi l_c^2}{a^2} \sqrt{1 - \sin^2 \gamma} \frac{1 + \cos \theta}{2} \right) \quad (15)$$

$\tilde{g}$  is the Zeeman parameter which is 60K for  $B \sim 45T$  and  $\cos \theta \equiv \hat{n}_1 \cdot \hat{n}_2$

$E_V$  is minimized at  $\gamma = 0$  or  $\gamma = \pi$ . Thus the nearest neighbour interaction picks out the  $Z_2$  broken,  $U(1)$  unbroken spin and charge ordered state (CDW) discussed

previously [8][11]. It is interesting to note that when the Dirac sea contributions are neglected ( $\mu = 1$ ),  $E_V$  is independent of the  $Q$ . This was also noticed by Alicea and Fisher [8]. They found that making the interactions slightly non-local picks out the  $\gamma = 0, \pi$  state.

The Hubbard term,  $E_U$ , does not contribute to the mean field energy if we neglect the contributions from the sea of filled Dirac-Landau levels. This can be qualitatively understood in the  $n = 0$  subspace. Since the two valley species live on the two distinct sub-lattices, if only one  $n = 0$  level is occupied, we can have any  $SU(4)$  polarization without any double occupancies. However, when the  $n \neq 0$  levels are taken into account,  $E_U$  is minimized when  $\theta = 0$  and  $\gamma = \pm\pi/2$ . The ground state is thus anti-ferromagnetic spin ordering (SDW) with the  $U(1)$  valley symmetry broken.

We need to minimise this energy density Eq.(15) with respect to the variational parameters  $\theta$ ,  $\gamma$  and  $m$ . Let us first consider the case when we ignore the Zeeman energy. The energy density minimizes for  $\gamma = 0, \pi$  (independent of  $\theta$ ) and  $\gamma = \pm\pi/2$  ( $\theta = 0$ ). The minimum energy is obtained at,

$$\gamma = 0(\pi) \text{ if } 3V - U > 0 ; \text{ any } \theta \quad (16)$$

$$\gamma = \frac{\pi}{2}(-\frac{\pi}{2}) \text{ if } 3V - U < 0 ; \theta = 0 \quad (17)$$

Thus at large  $V$  we have the  $Z_2$  broken,  $U(1)$  unbroken, spin polarised state and at large  $U$  we have the  $Z_2$  unbroken,  $U(1)$  broken, anti-ferromagnetic phase. The transition between them is first order and occurs at  $3V = U$  (at mean field level). The phase diagram is shown in inset of Fig.(2)

The minimization of energy density Eq.(15), yields same two phases in the  $V$ - $U$  space discussed above. The masses in the two phases are given by

$$m_{CDW} = \frac{a^2}{2\pi l_c^2} \frac{3V}{4} \left( 1 - \frac{3V}{2\tilde{t}} \right)^{-1} \quad (18)$$

$$m_{SDW} = \frac{a^2}{2\pi l_c^2} \frac{(3V + U)}{8} \left( 1 - \frac{3V + U}{4\tilde{t}} \right)^{-1} \quad (19)$$

The transition remains first order and the line separating two phases is given by the solution of

$$\frac{\left( \frac{3V+U}{4\tilde{t}} \right)^2}{1 - \frac{3V+U}{4\tilde{t}}} - \frac{\left( \frac{3V}{2\tilde{t}} \right)^2}{1 - \frac{3V}{4\tilde{t}}} = \frac{2\tilde{g}}{\tilde{t}} \frac{2\pi l_c^2}{a^2} \quad (20)$$

Note that to leading order in  $a/l_c$ , the phase boundary is independent of the magnetic field. In general we expect a weak magnetic field dependence.

The resulting phase diagram for the  $\nu = \pm 1$  is shown in Fig.(2). Thus at large  $U$  the Dirac sea polarization effects can drive the system into a  $U(1)$  valley symmetry

broken anti-ferromagnetic phase. Since the total spin polarization of this state is zero, the gap will have no dependence on the parallel component of the magnetic field in this phase, which is consistent with the recent experiments [1]. We therefore have a possible mechanism to explain the tilted field experiments at filling factors  $\nu = \pm 1$  [1]. It has been argued earlier, the Hubbard  $U$  drives the system towards anti-ferromagnetic order [14]. It can be seen from the Fig(2) that the estimate for the critical Hubbard  $U$  ( $\sim 15$  eV) is large. This number could change by including higher order corrections in  $a/l_c$  and the fluctuations about the mean field. Correlations may also be important even at the integer fillings [15] [16].

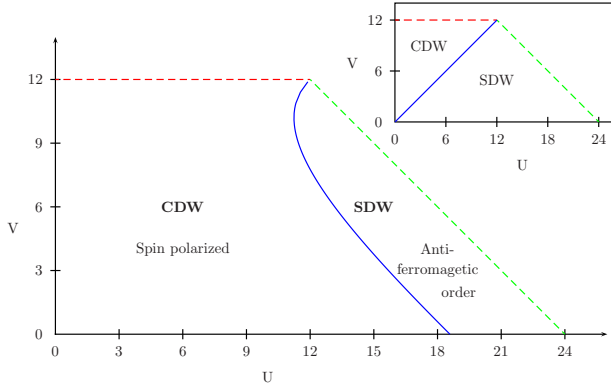


FIG. 2: The figure shows the phase diagram for  $\nu = \pm 1$  in the presence of the Zeeman term. The inset shows the phase diagram for the case when the Zeeman term is neglected. The CDW region,  $Z_2$  part of the valley symmetry is broken. In the SDW region,  $U(1)$  part of the valley symmetry is broken. All energies are in eV.

As we mentioned earlier, the dominant interaction in graphene is the  $SU(4)$  symmetric long range part of the Coulomb repulsion. As shown by Yang et. al. [7], this interaction favours  $SU(4)$  “ferromagnetic” order by the direct exchange mechanism. The  $SU(4)$  ferromagnetic order is quantified by the value of  $\langle \Psi_{\eta\sigma}^\dagger \Psi_{\eta'\sigma'} \rangle$ . As can be seen from equation (9), this is non-zero for the variational states we are considering. It is in fact independent of  $m$  because it gets contributions only from the  $n = 0$  levels. Thus the dominant gap in graphene will come from the the Coulomb exchange interaction which is proportional to  $\sqrt{B_\perp}$ .

The variational states also have an  $SU(4)$  “anti-ferromagnetic” order corresponding to a staggering at the scale of the lattice spacing. This is quantified by the value of  $\langle \tilde{\Psi}_{\eta\sigma} \Psi_{\eta'\sigma'} \rangle$ . Equation (10) shows that this is the component that is enhanced by a non-zero value of  $m$ . However at the scale of  $l_c$  over which the exchange mechanism operates, the effects of this order which varies at the scale of  $a$  will be small. The dominant gap will therefore be the “ferromagnetic” gap discussed above which is proportional to  $\sqrt{B_\perp}$ .

Thus we have shown that if among the short-range part of the interactions, the Hubbard interaction is dominant, then graphene has a  $U(1)$  valley symmetry broken phase with zero spin polarization at  $\nu = 1$ . The gap in this phase is proportional to  $\sqrt{B_\perp}$ . This phase is therefore consistent with the experimental results reported [1] where it is seen that the gap varies as  $\sqrt{B_\perp}$  and is independent of  $B_\parallel$ .

There will be three gapless collective modes in this phase. Two corresponding to the  $SU(2) \rightarrow U(1)$  spin symmetry breaking and one corresponding to the  $U(1)$  valley symmetry breaking. The topological defects in this phase are clearly interesting objects to study.

We have also analysed the  $\nu = 0$  phase in detail. The state is now parameterised by two orthogonal  $SU(4)$  spinors with ten parameters corresponding to the  $U(4)/(U(2) \times U(2))$  ground state manifold. The results will be reported in a longer forthcoming publication along with more details of the results reported in this letter.

**Acknowledgement:** We thank G. Baskaran for many useful discussions.

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